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Physical Chemistry Chemical Physics

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ISSN 1463-9076



PAPER

W. Kunz, M. Kellermeier *et al.*

Diffusion and precipitation processes in iron-based silica gardens

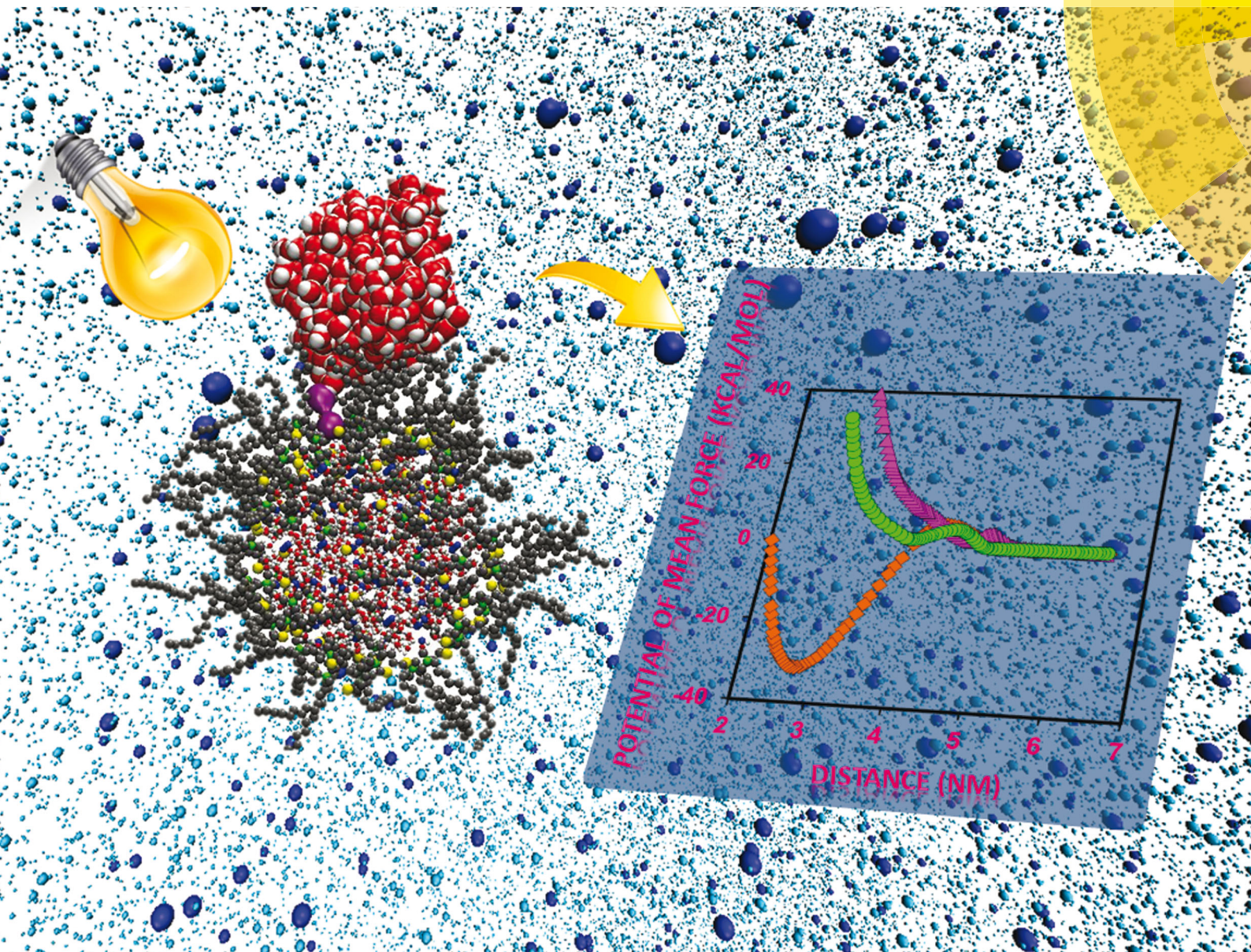
**175** YEARS



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PAPER

Alberto Striolo *et al.*

Molecular mechanisms responsible for hydrate anti-agglomerant performance

**175** YEARS



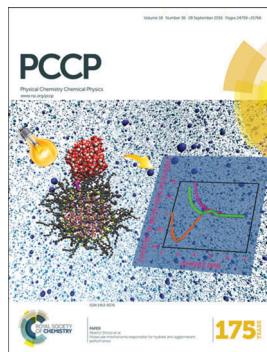
## IN THIS ISSUE

ISSN 1463–9076 CODEN PPCPFQ 18(36) 24759–25766 (2016)



### Cover

See W. Kunz, M. Kellermeier *et al.*, pp. 24850–24858. Image reproduced by permission of M. Kellermeier from *Phys. Chem. Chem. Phys.*, 2016, **18**, 24850.



### Inside cover

See Alberto Striolo *et al.*, pp. 24859–24871. Image reproduced by permission of Alberto Striolo from *Phys. Chem. Chem. Phys.*, 2016, **18**, 24859.

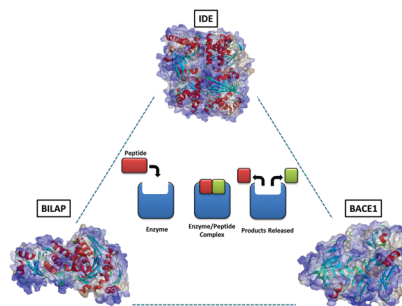
## PERSPECTIVES

24790

### Mechanisms of peptide hydrolysis by aspartyl and metalloproteases

Thomas J. Paul, Arghya Barman, Mehmet Ozbil, Ram Prasad Bora, Tingting Zhang, Gaurav Sharma, Zachary Hoffmann and Rajeev Prabhakar\*

Peptide hydrolysis has been involved in a wide range of biological, biotechnological, and industrial applications.

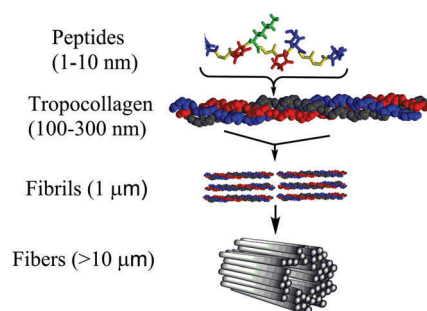


24802

### A perspective on structural and computational work on collagen

Carmen Domene,\* Christian Jorgensen and Sumra Wajid Abbasi

Collagen is the single most abundant protein in the extracellular matrix in the animal kingdom, with remarkable structural and functional diversity and regarded one of the most useful biomaterials.



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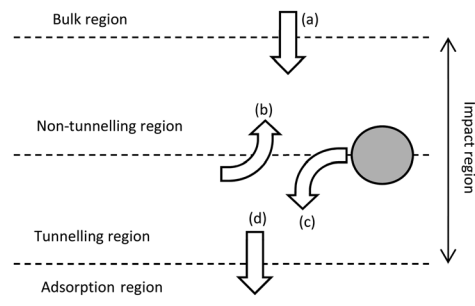
## PERSPECTIVES

24812

## Nanoparticle electrochemistry

Peter H. Robbs and Neil V. Rees\*

This perspective article provides a survey of recent advances in nanoscale electrochemistry, with a brief theoretical background and a detailed discussion of experimental results of nanoparticle based electrodes, including the rapidly expanding field of “impact electrochemistry”.



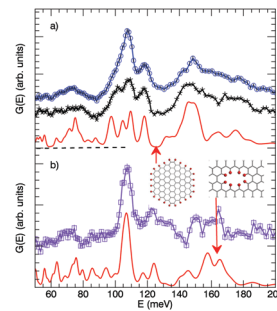
## COMMUNICATIONS

24820

## Hydrogen motions in defective graphene: the role of surface defects

Chiara Cavallari, Daniele Pontiroli, Mónica Jiménez-Ruiz, Mark Johnson, Matteo Aramini, Mattia Gaboardi, Stewart F. Parker, Mauro Riccò and Stéphane Rols\*

Understanding the mobility of H at the surface of carbon nanostructures is one of the essential ingredients for a deep comprehension of the catalytic formation of  $H_2$  in interstellar clouds.

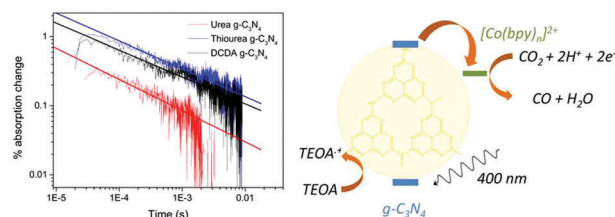


24825

Photochemical  $CO_2$  reduction using structurally controlled  $g-C_3N_4$ 

James J. Walsh, Chaoran Jiang, Junwang Tang\* and Alexander J. Cowan\*

Urea derived  $g-C_3N_4$  is a highly active  $CO_2$  reduction photocatalyst due to the location and driving force of photogenerated charges.

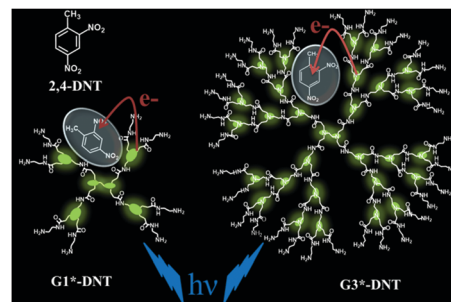


24830

## The study of electron transfer reactions in a dendrimeric assembly: proper utilization of dendrimer fluorescence

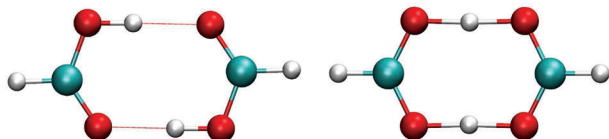
Somnath Koley and Subhadip Ghosh\*

Sensing applications of dendrimers: trapping of explosive nitroaromatic compounds within the dendrimer-cage followed by efficient quenching of its fluorescence.



## COMMUNICATIONS

24835

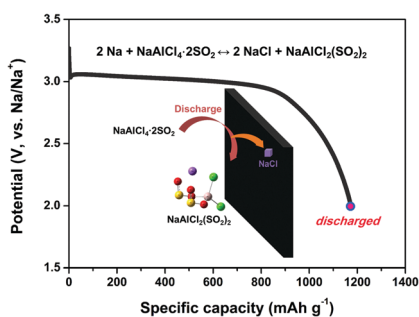


**An *ab initio* potential energy surface for the formic acid dimer: zero-point energy, selected anharmonic fundamental energies, and ground-state tunneling splitting calculated in relaxed 1–4-mode subspaces**

Chen Qu and Joel M. Bowman\*

We report a full-dimensional, permutationally invariant potential energy surface (PES) for the cyclic formic acid dimer.

24841

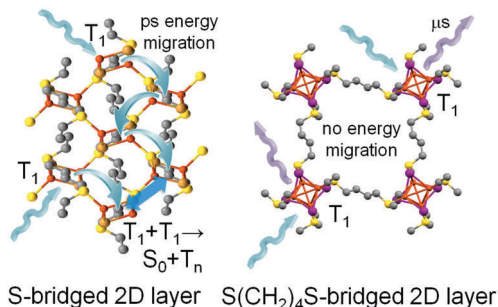


**A joint experimental and theoretical determination of the structure of discharge products in Na–SO<sub>2</sub> batteries**

Young-Kyu Han,\* Goojin Jeong, Keon-Joon Lee, Taeun Yim\* and Young-Jun Kim\*

This work is the first to elucidate the governing mechanism of molten-salt batteries by combining experimental and theoretical NMR measurements.

24845



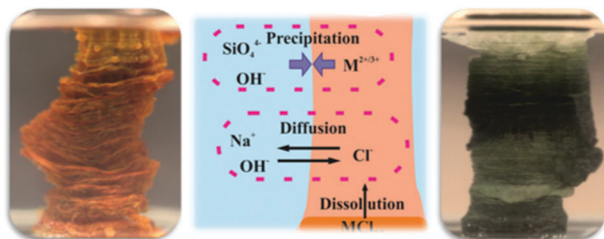
**The 3D [(Cu<sub>2</sub>Br<sub>2</sub>){μ-EtS(CH<sub>2</sub>)<sub>4</sub>SEt}]<sub>n</sub> material: a rare example of a coordination polymer exhibiting triplet–triplet annihilation**

Antoine Bonnot, Paul-Ludovic Karsenti, Frank Juvenal, Christopher Golz, Carsten Strohmman, Daniel Fortin, Michael Knorr\* and Pierre D. Harvey\*

A very rare case of excitation energy migration has been observed for an inorganic material.

## RESEARCH PAPERS

24850



**Diffusion and precipitation processes in iron-based silica gardens**

F. Glaab, J. Rieder, J. M. García-Ruiz, W. Kunz\* and M. Kellermeier\*

The time-dependent dynamic evolution of macroscopic silica garden tubes is shown to strongly depend on the used metal cations.



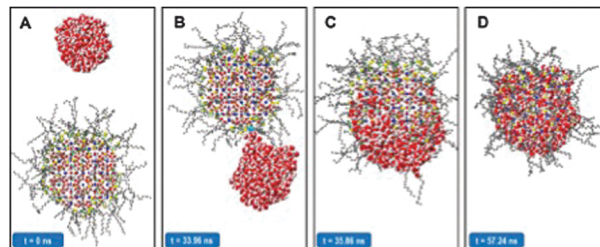
## RESEARCH PAPERS

24859

**Molecular mechanisms responsible for hydrate anti-agglomerant performance**

Anh Phan, Tai Bui, Erick Acosta, Pushkala Krishnamurthy and Alberto Striolo\*

Steered and equilibrium molecular dynamics simulations were employed to study the coalescence of a sl hydrate particle and a water droplet within a hydrocarbon mixture.

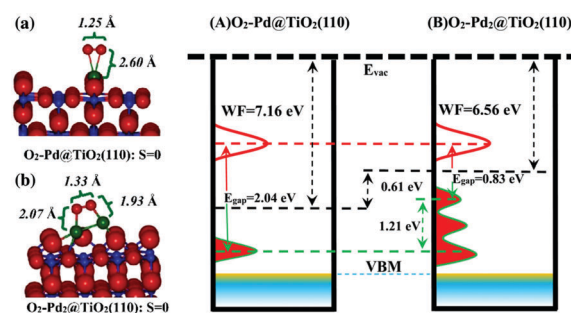


24872

**Interplay between the spin-selection rule and frontier orbital theory in O<sub>2</sub> activation and CO oxidation by single-atom-sized catalysts on TiO<sub>2</sub>(110)**

Shunfang Li, Xingju Zhao, Jinlei Shi, Yu Jia, Zhengxiao Guo, Jun-Hyung Cho,\* Yanfei Gao and Zhenyu Zhang\*

Distinct chemical activities of a Pd monomer and a Pd<sub>2</sub> dimer supported on TiO<sub>2</sub>(110) for O<sub>2</sub> activation.

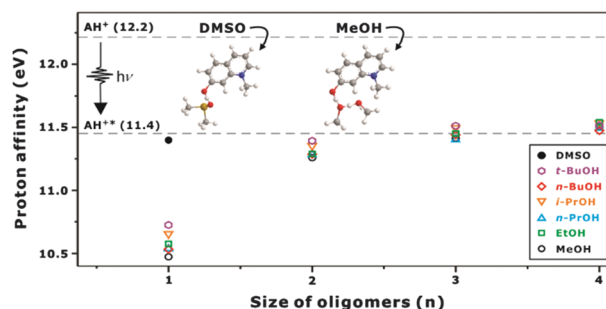


24880

**The critical size of hydrogen-bonded alcohol clusters as effective Brønsted bases in solutions**

Sun-Young Park, Taeg Gyum Kim, Manjaly J. Ajitha, Kijeong Kwac, Young Min Lee, Heesu Kim, Yousung Jung\* and Oh-Hoon Kwon\*

Hydrogen-bonded clustering of alcohol molecules increases their basicity (proton affinity) significantly, so that alcohol dimers can accept a proton which otherwise is impossible due to insufficient basicity as a monomer.

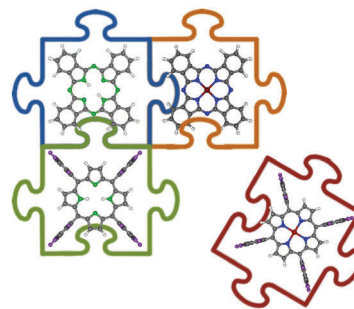


24890

**Electronic structure of CuTPP and CuTPP(F) complexes: a combined experimental and theoretical study II**

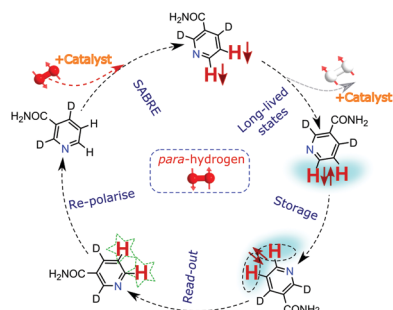
Giulia Mangione, Mauro Sami, Silvia Carlotto, Andrea Vittadini, Giovanni Ligorio, Melanie Timpel, Luca Pasquali, Angelo Giglia, Marco Vittorio Nardi and Maurizio Casarin\*

CuTPP and CuTPP(F) thick films deposited on Au(111) have been studied by coupling NEXAFS spectroscopy at the C/N/F K-edges and Cu L<sub>2,3</sub>-edges and spin-unrestricted TD-DFT calculations.



## RESEARCH PAPERS

24905

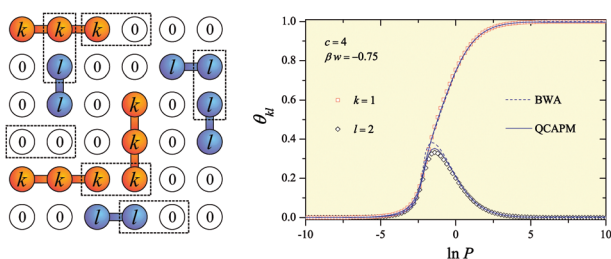


### Long-lived states to sustain SABRE hyperpolarised magnetisation

Soumya S. Roy, Peter J. Rayner, Philip Norcott, Gary G. R. Green and Simon B. Duckett\*

More than 4% net <sup>1</sup>H-polarisation is created, in seconds, that is detectable for over 2 minutes.

24912

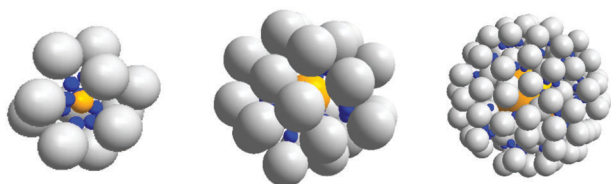


### Quasi-chemical approximation for polyatomic mixtures

M. V. Dávila,\* P. M. Pasinetti,\* D. A. Matoz-Fernandez and A. J. Ramirez-Pastor

The statistical thermodynamics of interacting binary mixtures of polyatomic species was developed.

24922

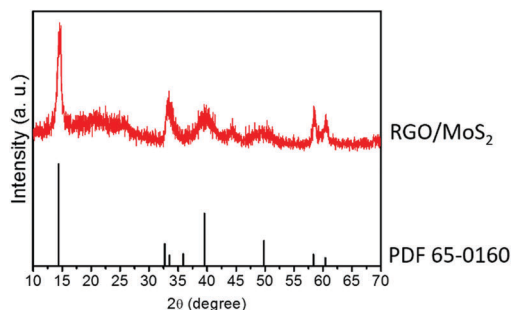


### Encapsulation of spherical nanoparticles by colloidal dimers

Gianmarco Munaò,\* Dino Costa, Santi Prestipino and Carlo Caccamo

Typical capsule structures resulting from the simulation of mixtures of colloidal dimers and spherical nanoparticles of variable size.

24931



### In situ growth of MoS<sub>2</sub> nanosheets on reduced graphene oxide (RGO) surfaces: interfacial enhancement of absorbing performance against electromagnetic pollution

Aming Xie, Mengxiao Sun, Kun Zhang, Wanchun Jiang, Fan Wu\* and Meng He\*

Electromagnetic pollution is rising all over the world.



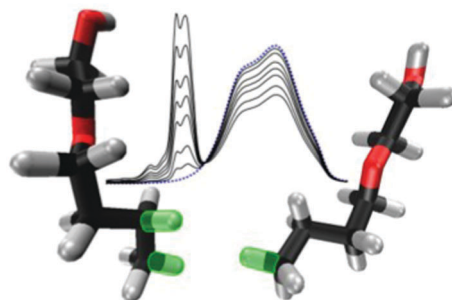
## RESEARCH PAPERS

24937

**Water-mediated aggregation of 2-butoxyethanol**

Shannon R. Pattenau, Blake M. Rankin, Kenji Mochizuki and Dor Ben-Amotz\*

Water plays an important role in mediating hydrophobic interactions, and yet important open questions remain regarding the magnitude, and even the sign, of water-mediated contributions to the potential of mean force between a pair of oily molecules dissolved in water.

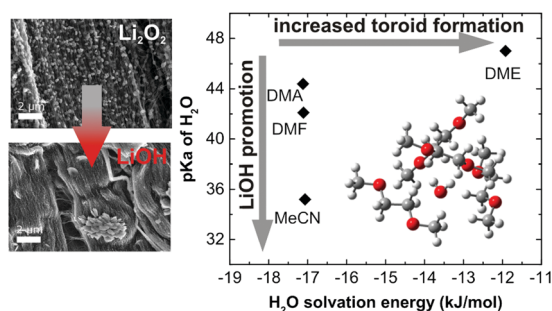


24944

**The effect of water on discharge product growth and chemistry in Li–O<sub>2</sub> batteries**

David G. Kwabi,\* Thomas P. Batcho, Shuting Feng, Livia Giordano, Carl V. Thompson and Yang Shao-Horn\*

Understanding what controls Li–O<sub>2</sub> battery discharge product chemistry and morphology is key to enabling its practical deployment as a low-cost, high-specific-energy energy conversion technology.

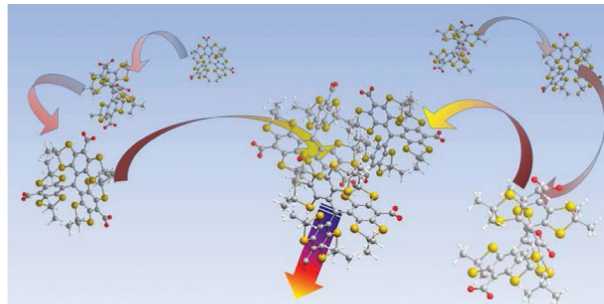


24954

**Electron spin dynamics and spin–lattice relaxation of trityl radicals in frozen solutions**

Hanjiao Chen, Alexander G. Maryasov, Olga Yu. Rogozhnikova, Dmitry V. Trukhin, Victor M. Tormyshev and Michael K. Bowman\*

Self-assembly of trityl radical aggregates dominates electron spin dynamics for dynamic nuclear polarization.

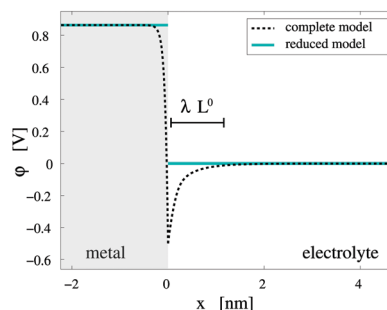


24966

**A new perspective on the electron transfer: recovering the Butler–Volmer equation in non-equilibrium thermodynamics**

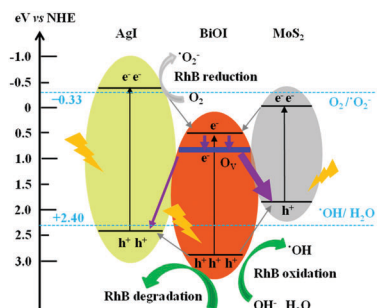
Wolfgang Dreyer, Clemens Gohlke and Rüdiger Müller\*

Butler–Volmer equations can be recovered from a complete non-equilibrium thermodynamic model by application of asymptotic analysis. Thereby we gain insight into the coupling of different physical phenomena and can derive Butler–Volmer equations for very different materials and electrochemical systems.



## RESEARCH PAPERS

24984

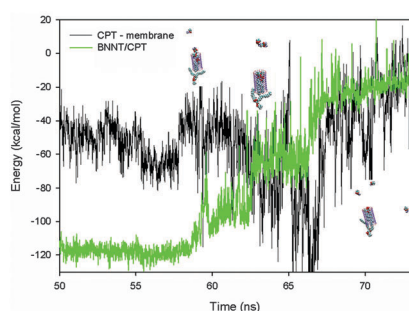


### An oxygen-vacancy rich 3D novel hierarchical MoS<sub>2</sub>/BiOI/AgI ternary nanocomposite: enhanced photocatalytic activity through photogenerated electron shuttling in a Z-scheme manner

M. Jahurul Islam, D. Amaranatha Reddy, Noh Soo Han, Jiha Choi, Jae Kyu Song\* and Tae Kyu Kim\*

Herein, we propose the photocatalytic mechanism, involving a Z-scheme and oxygen vacancy states, for the MoS<sub>2</sub>/BiOI/AgI nanocomposite.

24994

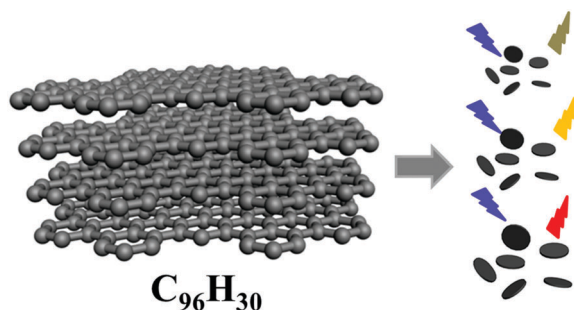


### Encapsulation capacity and natural payload delivery of an anticancer drug from boron nitride nanotube

M. El Khalifi, J. Bentin, E. Duverger, T. Gharbi, H. Boulahdour and F. Picaud\*

Payload delivery of anticancer cisplatin molecules assisted by the cell membrane lipid.

25002

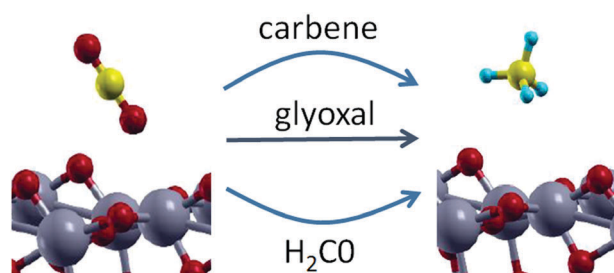


### C<sub>96</sub>H<sub>30</sub> tailored single-layer and single-crystalline graphene quantum dots

Biao Yuan, Xingming Sun, Jun Yan, Zheng Xie,\* Ping Chen and Shuyun Zhou\*

C<sub>96</sub>H<sub>30</sub> can be the precursor of single-layer and single-crystalline graphene quantum dots with a size-dependent effect.

25010



### A computational study of the competing reaction mechanisms of the photo-catalytic reduction of CO<sub>2</sub> on anatase(101)

Chung Man Ip and Alessandro Troisi\*

Three reaction pathways for the photocatalytic reduction of carbon dioxide to methane are investigated with density functional theory calculations.



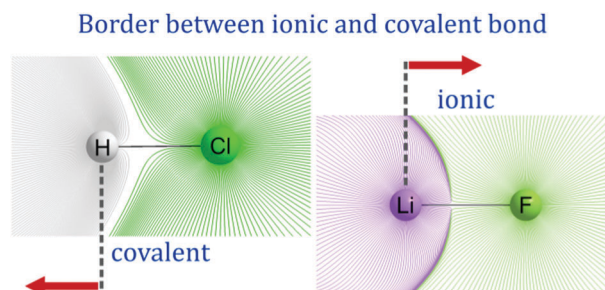
## RESEARCH PAPERS

25022

**Feynman force components: basis for a solution to the covalent vs. ionic dilemma**

Justyna Dominikowska,\* Mirosław Jabłoński and Marcin Palusiak

Feynman force components give fundamentals for distinction between covalent and ionic bonds without referring to the electronegativity concept.

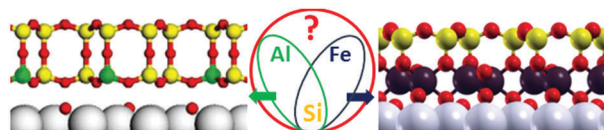


25027

**Preparation and structure of Fe-containing aluminosilicate thin films**

Héloïse Tissot, Linfei Li, Shamil Shaikhutdinov\* and Hans-Joachim Freund

Fe-containing aluminosilicate thin films exhibit a phase separation, which makes the formation of in-frame Fe in aluminosilicates (zeolites) unfavourable.

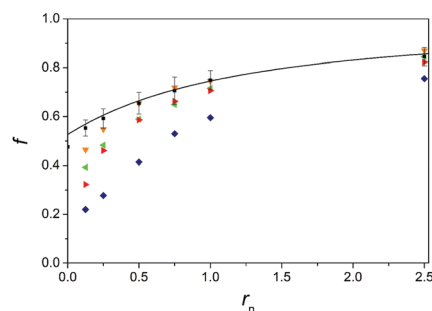


25036

**Influence of counterions on the conformation of conjugated polyelectrolytes: the case of poly(thiophen-3-ylacetic acid)**

Gregor Hostnik, Matjaž Bončina, Caterina Dolce, Guillaume Mériguet, Anne-Laure Rollet and Janez Cerar\*

Binding of large hydrophobic counterions to poly(thiophen-3-ylacetate) provokes the conformational change of this conjugated polyelectrolyte.

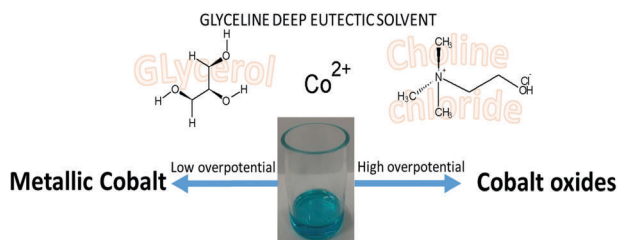


25048

**On the cobalt and cobalt oxide electrodeposition from a glyceline deep eutectic solvent**

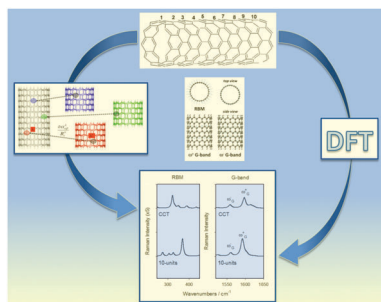
Alan M. P. Sakita, Rodrigo Della Noce, Cecilio S. Fugivara and Assis V. Benedetti\*

The electrodeposition of cobalt and cobalt oxides from a glyceline deep eutectic solvent is reported.



## RESEARCH PAPERS

25058

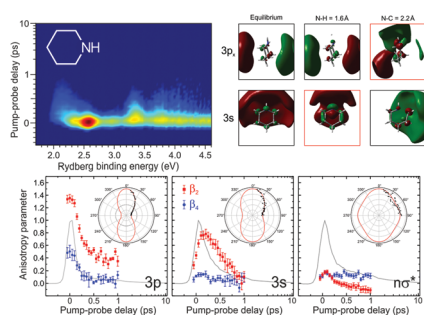


### Calculation of Raman parameters of real-size zigzag ( $n, 0$ ) single-walled carbon nanotubes using finite-size models

Teobald Kupka,\* Michal Stachów, Leszek Stobiński and Jakub Kaminsky\*

Structural and selected Raman features of real-size single-walled carbon nanotubes (SWCNTs) were studied using finite-size pristine SWCNT models at the DFT level.

25070

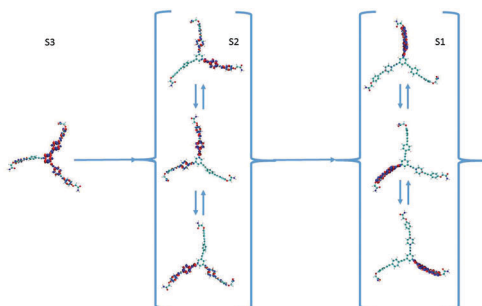


### Ultrafast relaxation dynamics of electronically excited piperidine: ionization signatures of Rydberg/valence evolution

Liv B. Klein, James O. F. Thompson, Stuart W. Crane, Lisa Saalbach, Theis I. Sølling, Martin J. Paterson and Dave Townsend\*

Time-resolved photoelectron spectroscopy reveals distinct ionization signatures of Rydberg-to-valence state evolution in the secondary aliphatic amine piperidine.

25080

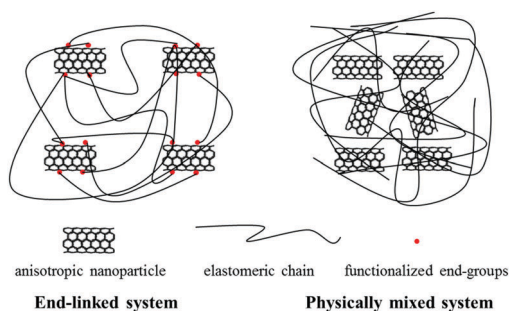


### Ultrafast electronic energy relaxation in a conjugated dendrimer leading to inter-branch energy redistribution

D. Ondarse-Alvarez, S. Kömürlü, A. E. Roitberg, G. Pierdominici-Sottile, S. Tretiak, S. Fernandez-Alberti\* and V. D. Kleiman\*

Dendrimers are arrays of coupled chromophores, where the energy of each unit depends on its structure and conformation.

25090



### Tuning the structure and mechanical property of polymer nanocomposites by employing anisotropic nanoparticles as netpoints

Zijian Zheng, Fanzhu Li, Hongji Liu, Jianxiang Shen, Jun Liu,\* Youping Wu,\* Liqun Zhang and Wenchuan Wang

We report a new kind of polymer nanocomposite by means of employing anisotropic nanoparticles as netpoints, to chemically connect the dual end-groups of each polymer chain to form a network.



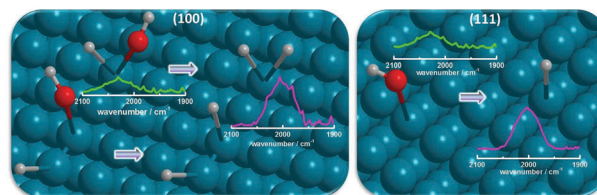
## RESEARCH PAPERS

25100

### Mechanism of the potential-triggered surface transformation of germanium in acidic medium studied by ATR-IR spectroscopy

Simantini Nayak and Andreas Erbe\*

During the electrochemical surface transformation of Ge(100) and Ge(111) surfaces from an –OH to an –H terminated surface, different potential dependent transient species are observed.

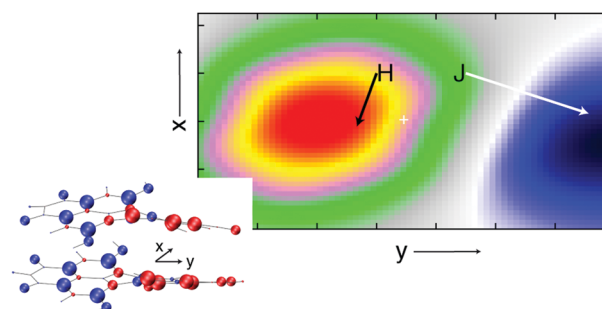


25110

### Biphasic aggregation of a perylene bisimide dye identified by exciton-vibrational spectra

P.-A. Plötz, S. P. Polyutov, S. D. Ivanov, F. Fennel, S. Wolter, T. Niehaus, Z. Xie, S. Lochbrunner, F. Würthner and O. Kühn\*

The quantum efficiency of light emission supramolecular aggregates strongly depends on the intermolecular coupling. We present a molecule which demonstrates two different aggregated structures with high and low quantum efficiency. The spectral signatures can be understood by simulating the aggregated structures and the corresponding exciton-vibrational spectra.

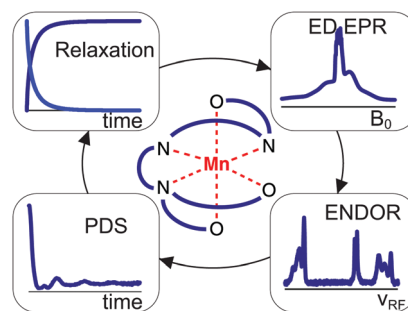


25120

### EPR characterization of Mn(II) complexes for distance determination with pulsed dipolar spectroscopy

Katharina Keller, Michal Zalibera, Mian Qi, Vanessa Koch, Julia Wegner, Henrik Hintz, Adelheid Godt,\* Gunnar Jeschke, Anton Savitsky\* and Maxim Yulikov\*

EPR properties of four Mn(II) complexes and Tikhonov regularization-based analysis of RIDME data containing dipolar overtones are presented.

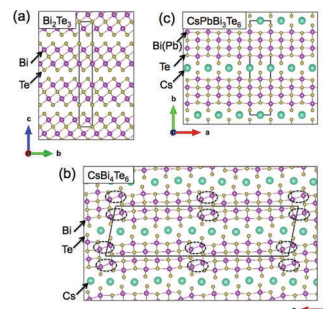


25136

### Determination of the local structure of CsBi<sub>4-x</sub>Pb<sub>x</sub>Te<sub>6</sub> (x = 0, 0.5) by X-ray absorption spectroscopy

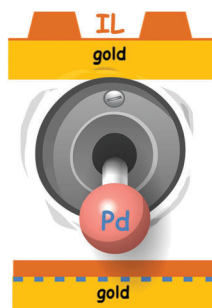
Takanori Wakita,\* Eugenio Paris, Takashi Mizokawa, Muammer Yasin Hacisalihoğlu, Kensei Terashima, Hiroyuki Okazaki, Olivier Proux, Isabelle Kieffer, Eric Lahera, William Del Net, Luca Olivi, Yoshihiko Takano, Yuji Muraoka, Takayoshi Yokoya and Naurang L. Saini

We have studied the local structure and valence electronic unoccupied states of CsBi<sub>4</sub>Te<sub>6</sub> and CsBi<sub>3.5</sub>Pb<sub>0.5</sub>Te<sub>6</sub> ( $T_c \sim 3$  K) by EXAFS and XANES measurements.



## RESEARCH PAPERS

25143

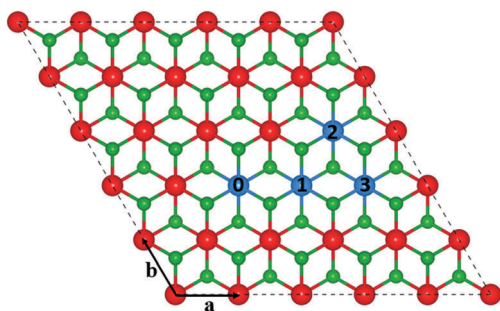


### Switching adsorption and growth behavior of ultrathin $[C_2C_1Im][OTf]$ films on Au(111) by Pd deposition

F. Rietzler, B. May, H.-P. Steinrück and F. Maier\*

*In vacuo* deposition of ultrathin ionic liquid films combined with angle-resolved X-ray photoelectron spectroscopy demonstrates that the initial three-dimensional growth mode of  $[C_2C_1Im][OTf]$  deposited onto the bare Au(111) surface can be switched to two-dimensional growth by adding submonolayer amounts of Pd.

25151

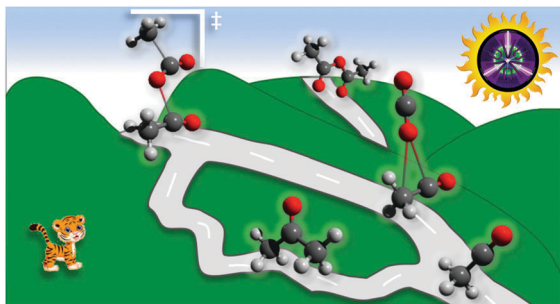


### Theoretical prediction of long-range ferromagnetism in transition-metal atom-doped $d^0$ dichalcogenide single layers $SnS_2$ and $ZrS_2$

L. Ao, A. Pham,\* H. Y. Xiao, X. T. Zu and S. Li

We have systematically investigated the effects of transition-metal (TM) atom (Sc–Zn) doping in 2D  $d^0$  materials  $SnS_2$  and  $ZrS_2$  via the density functional theory method.

25161

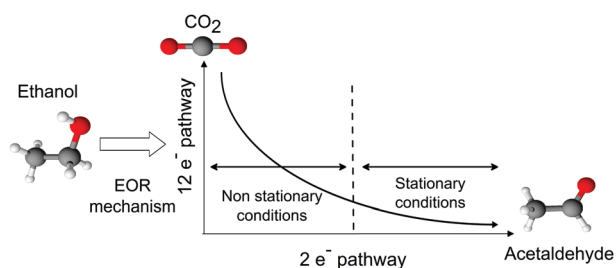


### Bifurcated dissociative photoionization mechanism of acetic acid anhydride revealed by imaging photoelectron photoion coincidence spectroscopy

Krisztina Voronova, Chrissa M. Mozaffari Easter, Krisztián G. Torma, Andras Bodi, Patrick Hemberger and Bálint Sztáray\*

PEPICO allows us a peek beyond the transition state to identify bifurcated reaction pathways.

25169



### The influence of mass-transport conditions on the ethanol oxidation reaction (EOR) mechanism of Pt/C electrocatalysts

Antoine Bach Delpeuch,\* Marjorie Jacquot, Marian Chatenet and Carsten Cremers

This study aims to provide further understanding of the influence of different parameters that control mass-transport (the revolution rate of the rotating disk electrode and the potential scan rate) on the ethanol oxidation reaction (EOR).

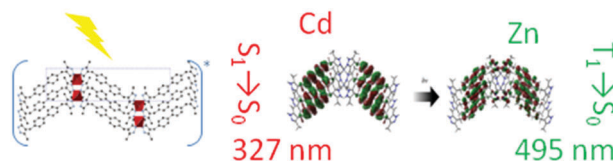
## RESEARCH PAPERS

25176

### Modelling photophysical properties of metal–organic frameworks: a density functional theory based approach

Liam Wilbraham, François-Xavier Coudert\* and Ilaria Ciofini\*

Photoluminescence of zinc and cadmium-based metal–organic frameworks has been characterized using density functional theory (DFT) and time-dependent DFT.

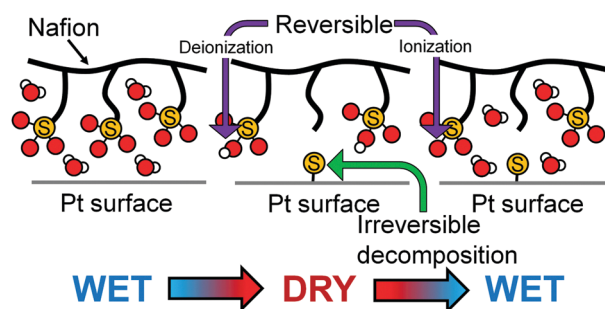


25183

### In situ S-K XANES study of polymer electrolyte fuel cells: changes in the chemical states of sulfonic groups depending on humidity

Kazuhisa Isegawa, Tetsuo Nagami, Shinji Jomori, Masaaki Yoshida and Hiroshi Kondoh\*

Changes in the chemical states of sulfonic groups of Nafion in polymer electrolyte fuel cells (PEFCs) under gas-flowing conditions were studied using *in situ* S-K XANES spectroscopy.

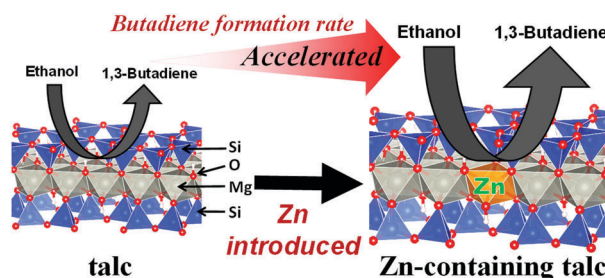


25191

### Experimental and computational studies of the roles of MgO and Zn in talc for the selective formation of 1,3-butadiene in the conversion of ethanol

Yoshihiro Hayashi, Sohta Akiyama, Akimitsu Miyaji, Yasumasa Sekiguchi, Yasuharu Sakamoto, Akinobu Shiga, To-ru Koyama, Ken Motokura and Toshihide Baba\*

The one-step conversion of ethanol to 1,3-butadiene was performed using talc containing Zn (talc/Zn) as a catalyst.

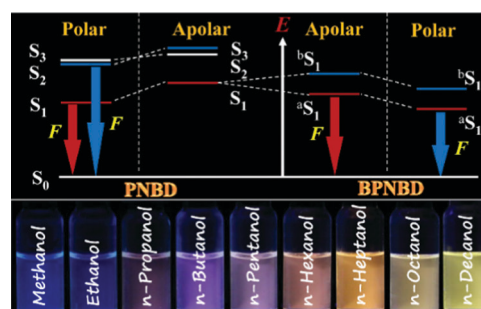


25210

### New solvatochromic probes: performance enhancement via regulation of excited state structures

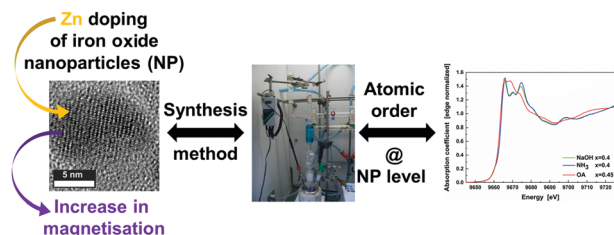
Huijing Liu, Xiaojie Xu, Haonan Peng, Xingmao Chang, Xuwei Fu, Qianshu Li, Shiwei Yin,\* Gary J. Blanchard\* and Yu Fang\*

Regulation of excited state structures resulted in new fluorophores with much enhanced solvatochromic properties.





25221

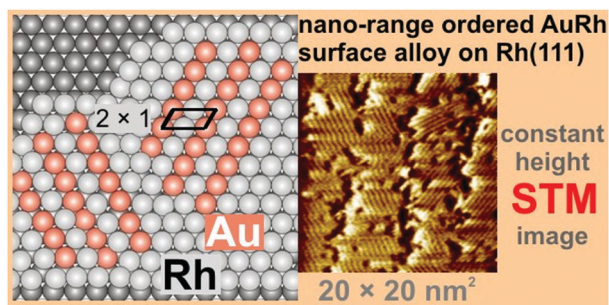


### Pushing up the magnetisation values for iron oxide nanoparticles *via* zinc doping: X-ray studies on the particle's sub-nano structure of different synthesis routes

Wojciech Szczerba,\* Jan Żukrowski, Marek Przybylski, Marcin Sikora, Olga Safonova, Aleksey Shmeliov, Valeria Nicolosi, Michael Schneider, Tim Granath, Maximilian Oppmann, Marion Straßer and Karl Mandel\*

We study how only slightly different synthesis approaches towards zinc doped iron oxide nanoparticles strongly influences the resulting structure and magnetisation.

25230

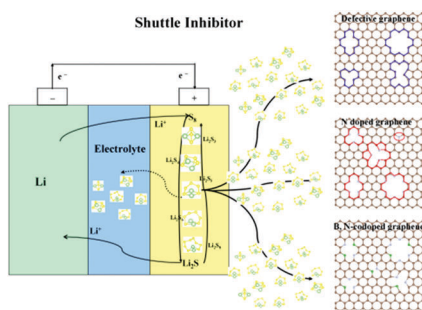


### The growth and thermal properties of Au deposited on Rh(111): formation of an ordered surface alloy

László Óvári,\* András Berkó,\* Gábor Vári, Richárd Gubó, Arnold Péter Farkas and Zoltán Kónya

Scanning tunnelling microscopy (STM), low energy ion scattering spectroscopy (LEIS), X-ray photoelectron spectroscopy (XPS) and high resolution electron energy loss spectroscopy (HREELS) were applied for studying Au deposited on the Rh(111) surface.

25241

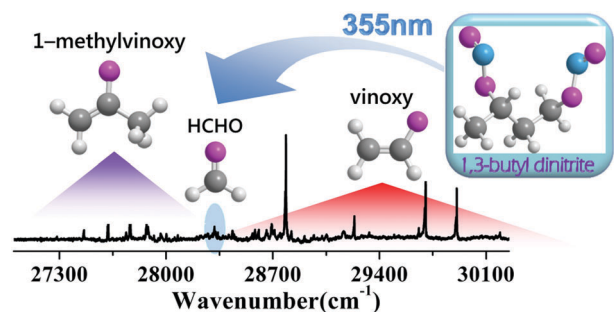


### Shuttle inhibition by chemical adsorption of lithium polysulfides in B and N co-doped graphene for Li-S batteries

Fen Li, Yan Su and Jijun Zhao\*

The shuttle effect can be effectively depressed by the synergistic contribution of  $N \cdots Li$  and  $B \cdots S$  interactions.

25249



### Photodissociation dynamics of dinitrite at 355 nm: initiation of a reactive pathway

Lingxuan Wang and Lily Zu\*

Vinoxyl and 1-methylvinoxyl radicals were detected along with formaldehyde as the products in the photodissociation of 1,3-butyl dinitrite.

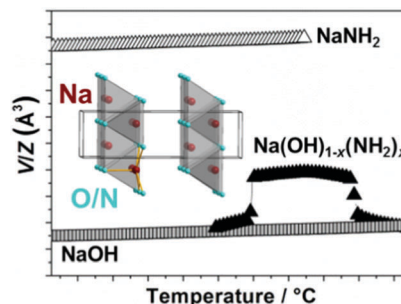
## RESEARCH PAPERS

25257

### Thermal decomposition of sodium amide, $\text{NaNH}_2$ , and sodium amide hydroxide composites, $\text{NaNH}_2\text{--NaOH}$

Lars H. Jepsen, Peikun Wang, Guotao Wu, Zhitao Xiong, Flemming Besenbacher, Ping Chen and Torben R. Jensen\*

Composites of  $\text{NaNH}_2$  and the omnipresent  $\text{NaOH}$  have a lower melting temperature and form a non-stoichiometric solid solution,  $\text{Na(OH)}_{1-x}(\text{NH}_2)_x$ , during heating.

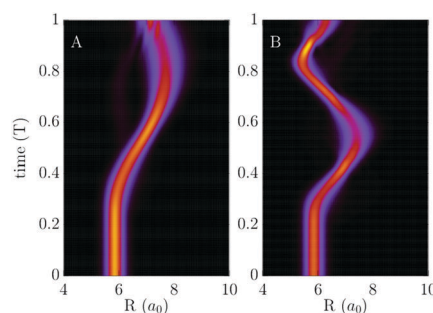


25265

### Nonresonant electronic transitions induced by vibrational motion in light-induced potentials

Pablo Sampedro, Bo Y. Chang and Ignacio R. Sola\*

We find a new mechanism of electronic population inversion using strong femtosecond pulses, where the transfer is mediated by vibrational motion on a light-induced potential.

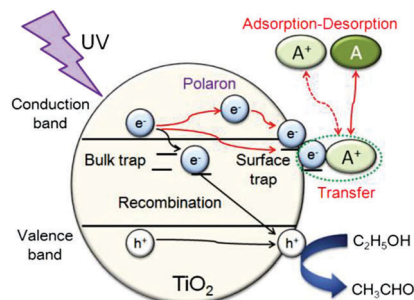


25271

### Distinction of electron pathways at titanium oxide/liquid interfaces in photocatalytic processes and co-catalyst effects

Shota Kuwahara and Kenji Katayama\*

The combination of the transient grating method and max entropy analysis revealed three different electron dynamics in the photocatalytic processes of co-catalyst/ $\text{TiO}_2$ , corresponding to intrinsic recombination and the decay of surface-trapped electrons and polarons.

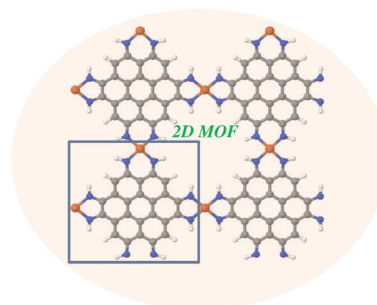


25277

### Coronene-based metal–organic framework: a theoretical exploration

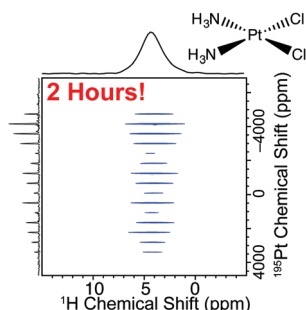
Chandrima Chakravarty, Bikash Mandal and Pranab Sarkar\*

A new coronene-based 2D metal–organic framework with interesting magnetic and electronic and remarkable spin-filtering properties has been proposed.



## RESEARCH PAPERS

25284

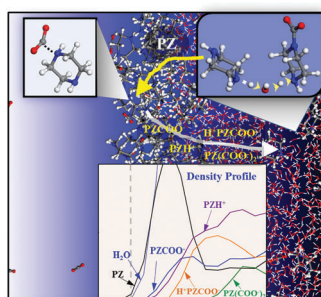


### Rapid acquisition of wideline MAS solid-state NMR spectra with fast MAS, proton detection, and dipolar HMQC pulse sequences

Aaron J. Rossini,\* Michael P. Hanrahan and Martin Thuo

Fast MAS and proton detection are applied to rapidly acquire wideline solid-state NMR spectra of spin-1/2 and half-integer quadrupolar nuclei.

25296

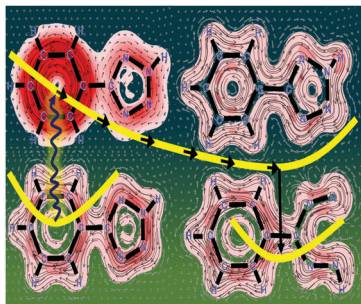


### First-principles assessment of CO<sub>2</sub> capture mechanisms in aqueous piperazine solution

Haley M. Stowe, Eunsu Paek and Gyeong S. Hwang\*

In this theoretical study, we elucidate molecular mechanisms underlying CO<sub>2</sub> absorption in aqueous piperazine (PZ) solution.

25308

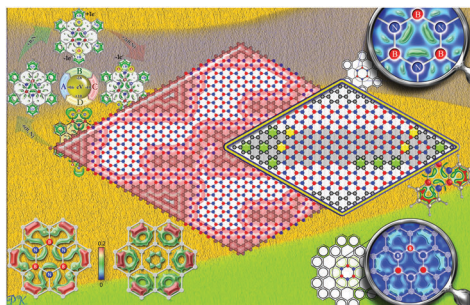


### Deciphering the cryptic role of a catalytic electron in a photochemical bond dissociation using excited state aromaticity markers

Ambar Banerjee, Debabrata Halder, Gaurab Ganguly and Ankan Paul\*

Upon photoexcitation of 5-phenyltetrazole, an electron is injected from the phenyl ring to the tetrazole ring, which performs a catalytic role in the photolytic dissociation of N<sub>2</sub>. The footprints of the "mercenary" electron are captured via dramatic changes in excited state aromaticity of the associated rings.

25315



### Establishing the pivotal role of local aromaticity in the electronic properties of boron-nitride graphene lateral hybrids

Nicolás Otero, Khaled E. El-kelany, Claude Pouchan, Michel Rérat and Panaghiotis Karamanis\*

Within an attempt to unravel the conundrum of irregular bandgap variations in hybrids of white-graphene (hBN) and graphene (G) observed in both experiment and theory, strong proofs about the decisive role of aromaticity in their electronic properties are brought to light.



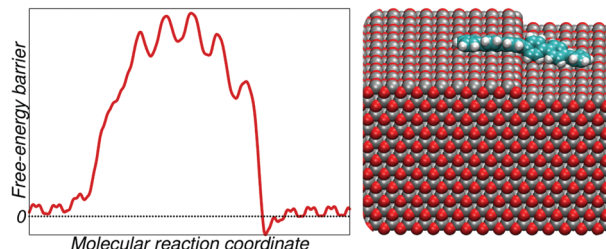
## RESEARCH PAPERS

25329

**Characterization of step-edge barrier crossing of *para*-sexiphenyl on the ZnO (1010) surface**

Karol Palczynski, Philipp Herrmann, Georg Heimel and Joachim Dzubiella\*

Mass transport processes of conjugated organic molecules (COMs) on inorganic surfaces are essential elements in thin film deposition for hybrid optoelectronic devices.

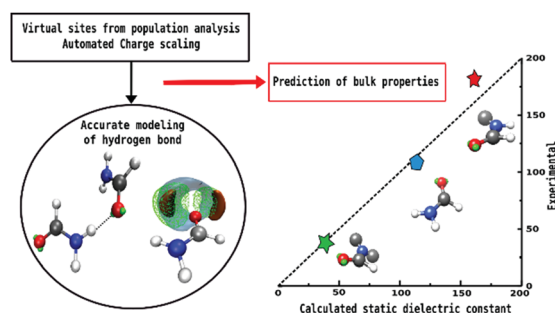


25342

**Accurate prediction of bulk properties in hydrogen bonded liquids: amides as case studies**

Marina Macchiagodena, Giordano Mancini,\* Marco Pagliai\* and Vincenzo Barone

Accurate tuning of polarization effects and generation of effective virtual sites allows bulk properties to be obtained in agreement with experimental values.

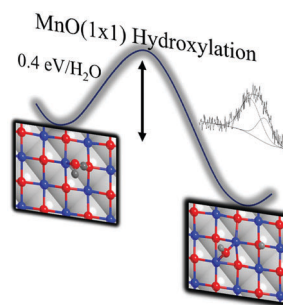


25355

**Water dissociation on MnO(1 × 1)/Ag(100)**

Chris Arble, Xiao Tong, Livia Giordano, Anna Maria Ferrari\* and John T. Newberg\*

MnO(1 × 1)/Ag(100) hydroxylation occurs at terrace sites for water monomers.

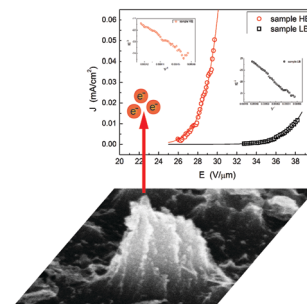


25364

**Nanoshaping field emitters from glassy carbon sheets: a new functionality induced by H-plasma etching**

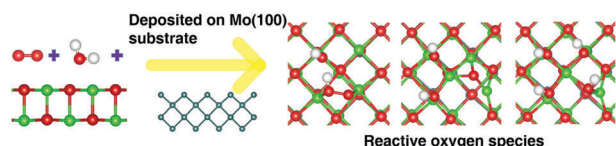
S. Gay, S. Orlanducci, D. Passeri,\* M. Rossi and M. L. Terranova

This paper reports on the morphological and electrical characterization at the nanometer scale and the investigation of the field emission characteristics of glassy carbon (GC) plates which underwent H-induced physical/chemical processes occurring in a dual-mode MW-RF plasma reactor.



## RESEARCH PAPERS

25373

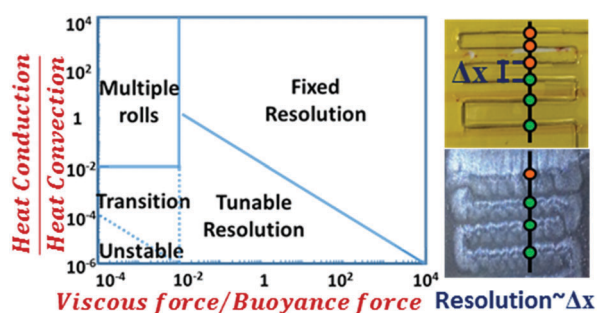


### Generation of highly reactive oxygen species on metal-supported MgO(100) thin films

Zhenjun Song, Jing Fan, Yueyue Shan,\*  
Alan Man Ching Ng\* and Hu Xu\*

A series of highly reactive oxygen species are formed with the assistance of water on an insulating surface.

25380

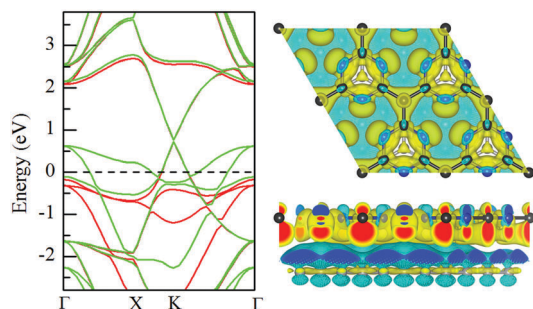


### The flow patterning capability of localized natural convection

Ling-Ting Huang and Ling Chao\*

Controlling flow patterns to align materials can have various applications in optics, electronics, and biosciences. We developed a natural-convection-based method to create desirable spatial flow patterns by controlling the locations of heat sources and proposed a flow pattern state diagram which suggests a suitable range of operating conditions for flow patterning.

25388

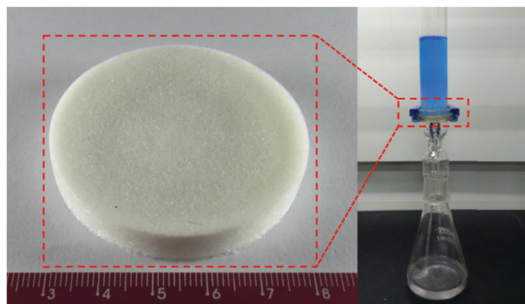


### A multifunctional material of two-dimensional g-C<sub>4</sub>N<sub>3</sub>/graphene bilayer

Jie Cui, Shuhua Liang\* and Jianmin Zhang

Using first-principles calculations, we present a multifunctional material of g-C<sub>4</sub>N<sub>3</sub>/graphene bilayer with great potentials in the field of spintronics and photocatalysis.

25394



### A robust salt-tolerant superoleophobic aerogel inspired by seaweed for efficient oil–water separation in marine environments

Yuqi Li, Hui Zhang, Mizi Fan,\* Jiandong Zhuang and Lihui Chen

A robust salt-tolerant superoleophobic aerogel was fabricated by a simple combined freeze-drying and ionic cross-linking method for oil–seawater separation.

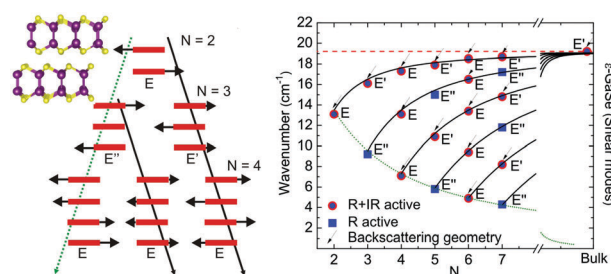
## RESEARCH PAPERS

25401

## Ultra-weak interlayer coupling in two-dimensional gallium selenide

R. Longuinhos and J. Ribeiro-Soares\*

By using symmetry arguments and first principles calculations, we study the stability of  $\beta$  and  $\epsilon$  few-layer GaSe and their low-frequency interlayer breathing and shear modes, unveiling uncommon lubricant properties and exfoliability at the nanoscale.

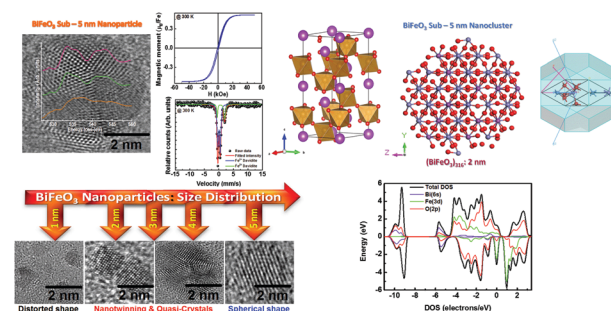


25409

Observation of nanotwinning and room temperature ferromagnetism in sub-5 nm BiFeO<sub>3</sub> nanoparticles: a combined experimental and theoretical study

Mandar M. Shirolkar,\* Xiaolei Dong, Jieni Li, Shiliu Yin, Ming Li and Haiqian Wang\*

The nanotwinning, covalent nature and magnetic properties of BiFeO<sub>3</sub> nanoparticles of sub-5 nm size are investigated.

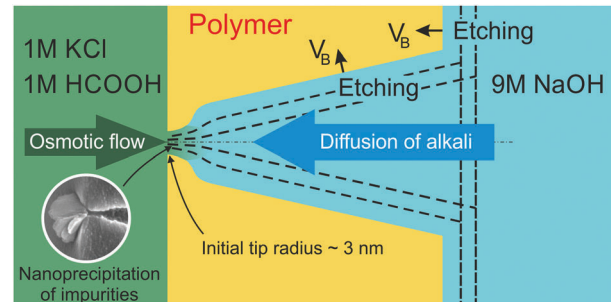


25421

## Shedding light on the mechanism of asymmetric track etching: an interplay between latent track structure, etchant diffusion and osmotic flow

Pavel Y. Apel,\* Valery V. Bashevoy, Irina V. Blonskaya, Nikolay E. Lizunov, Oleg L. Orelovitch and Christina Trautmann

Asymmetric etching of ion tracks is strongly affected by osmotic flow which has a determinative effect on nanopore geometry. As a result, the narrowest part of the pore evolves through a variety of configurations.

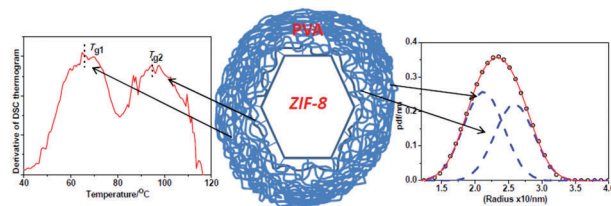


25434

## Unraveling the sub-nanosopic structure at interphase in a poly(vinyl alcohol)–MOF nanocomposite, and its role in thermo-mechanical properties

S. K. Sharma, K. Sudarshan and P. K. Pujari\*

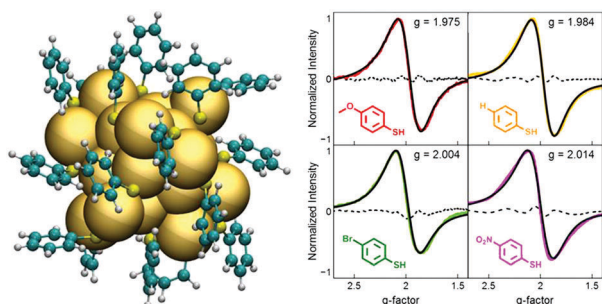
Polymer chain framework at the interfacial region in PVA–MOF nanocomposites can be represented by a rigid but rather open network.





## RESEARCH PAPERS

25443

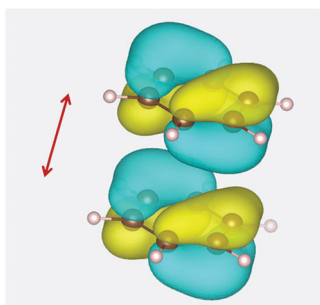


### Probing ligand-induced modulation of metallic states in small gold nanoparticles using conduction electron spin resonance

Anthony Cirri, Alexey Silakov, Lasse Jensen and Benjamin J. Lear\*

We acquire conduction electron spin resonance spectra for small gold nanoparticles protected by a series of *para*-substituted thiophenol ligands. Our results demonstrate that changes in ligand identity affect the quantum mechanical behavior of electrons within the nanoparticle's metallic core.

25452

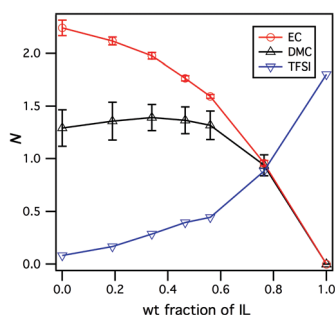


### A new insight into $\pi$ - $\pi$ stacking involving remarkable orbital interactions

Rundong Zhao and Rui-Qin Zhang\*

The importance of orbital interaction in  $\pi$ - $\pi$  interactions is explored in detail and a unified description of  $\pi$ - $\pi$  stacking is proposed.

25458

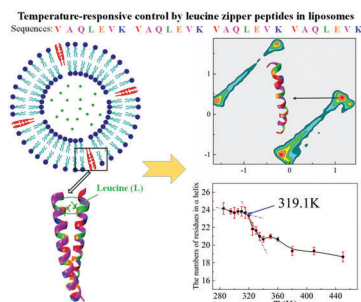


### Enhanced low-temperature ionic conductivity via different $\text{Li}^+$ solvated clusters in organic solvent/ionic liquid mixed electrolytes

Luis Aguilera, Johan Scheers and Aleksandar Matic\*

We investigate  $\text{Li}^+$  coordination in mixed electrolytes based on ionic liquids (ILs) and organic solvents and its relation with the macroscopic properties such as phase behaviour and ionic conductivity.

25465



### Computational insights into the destabilization of $\alpha$ -helical conformations formed by leucine zipper peptides in response to temperature

Xiejun Xu, Xingqing Xiao, Shouhong Xu and Honglai Liu\*

The computed transition temperature of leucine zipper peptides is 319.1 K, which is in quantitative agreement with the experimental measurement, 321.1 K.

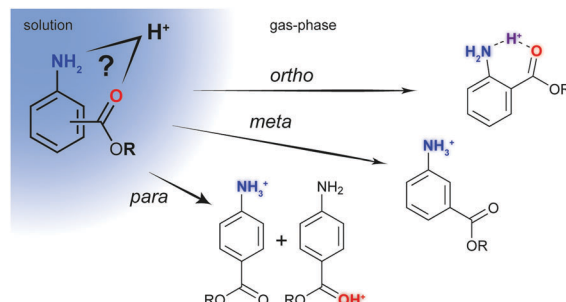
## RESEARCH PAPERS

25474

### The impact of environment and resonance effects on the site of protonation of aminobenzoic acid derivatives

Jongcheol Seo, Stephan Warnke, Sandy Gewinner, Wieland Schöllkopf, Michael T. Bowers, Kevin Pagel\* and Gert von Helden\*

Ion mobility- and  $m/z$ -selected infrared spectroscopy unambiguously determines the site of protonation of  $p$ -,  $m$ -, and  $o$ -aminobenzoic acid derivatives.

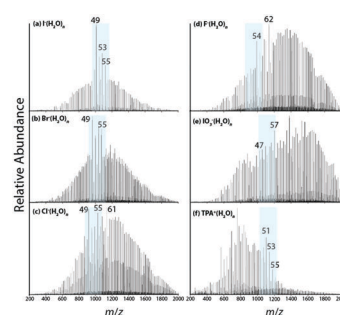


25483

### The effect of halide and iodate anions on the hydrogen-bonding network of water in aqueous nanodrops

Satrajit Chakrabarty and Evan R. Williams\*

The hydration of halide and iodate anions was investigated using electrospray ionization (ESI) mass spectrometry and infrared photodissociation (IRPD) spectroscopy.

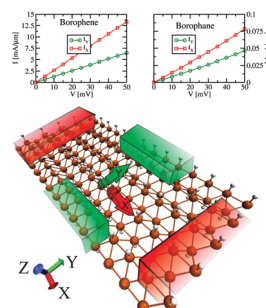


25491

### Directional dependence of the electronic and transport properties of 2D borophene and borophane

José Eduardo Padilha,\* Roberto Hiroki Miwa and Adalberto Fazzio

Borophene and borophane present directional dependency on the electronic transport properties which could be tuned by an external anisotropic strain.

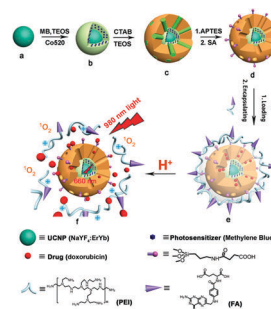


25497

### pH-Responsive drug release and NIR-triggered singlet oxygen generation based on a multifunctional core-shell-shell structure

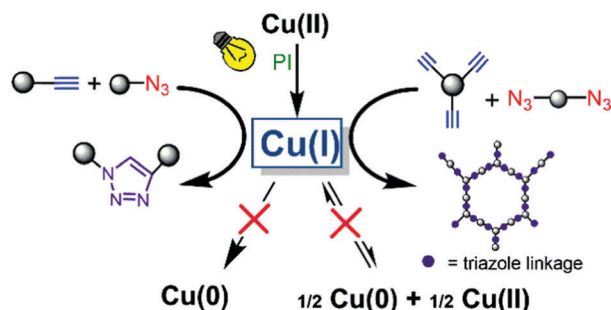
Renlu Han, Haopeng Yi, Junhui Shi, Zongjun Liu, Hao Wang, Yafei Hou and You Wang\*

A multifunctional platform drug with pH-responsive drug release and near-infrared (NIR) light-triggered photodynamic therapy (PDT) was designed and prepared using the novel core-shell-shell structure.



## RESEARCH PAPERS

25504

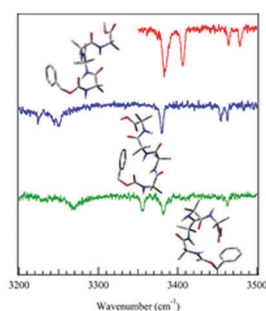


### Towards understanding the kinetic behaviour and limitations in photo-induced copper(I) catalyzed azide-alkyne cycloaddition (CuAAC) reactions

Bassil M. El-Zaatari, Abhishek U. Shete, Brian J. Adzima and Christopher J. Kloxin\*

The kinetics of the photo-CuAAC reaction were studied in various systems (monofunctional and polymer), providing new mechanistic and behavioral insight.

25512

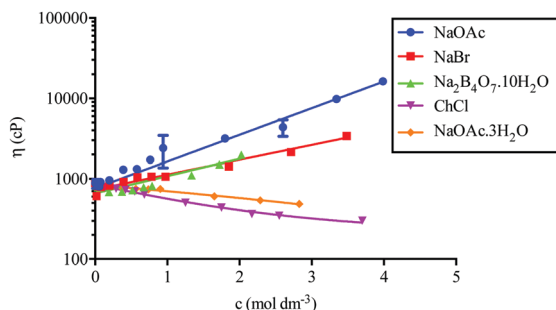


### Conformation-specific spectroscopy of capped, gas-phase Aib oligomers: tests of the Aib residue as a 3<sub>10</sub>-helix former

Joseph R. Gord, Daniel M. Hewett, Alicia O. Hernandez-Castillo, Karl N. Blodgett, Matthew C. Rotondaro, Adalgisa Varuolo, Matthew A. Kubasik\* and Timothy S. Zwier\*

Single-conformation spectroscopy is used to probe the preference for helical structural in Aib-homopeptides.

25528

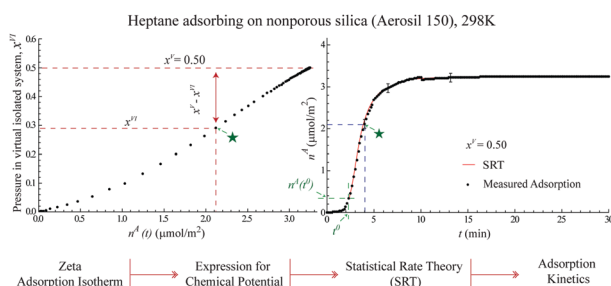


### Do group 1 metal salts form deep eutectic solvents?

A. P. Abbott,\* C. D'Agostino,\* S. J. Davis, L. F. Gladden and M. D. Mantle

Group 1 salts were compared with quaternary ammonium chlorides for their ability to form deep eutectic solvents and it was found that while some formed liquids the sodium ions caused the liquids to become structured and increased their viscosity.

25538



### Vapour adsorption kinetics: statistical rate theory and zeta adsorption isotherm approach

Seyed Hadi Zandavi and C. A. Ward\*

The zeta adsorption isotherm may be combined with statistical rate theory to formulate an expression for vapour adsorption kinetics that is in terms of a rate constant. For heptane adsorbing on silica, the rate constant is experimentally shown to depend only on temperature.



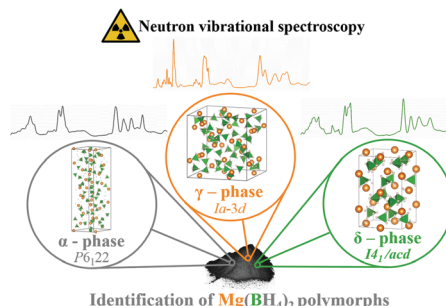
## RESEARCH PAPERS

25546

### Structure-dependent vibrational dynamics of $\text{Mg}(\text{BH}_4)_2$ polymorphs probed with neutron vibrational spectroscopy and first-principles calculations

Mirjana Dimitrievska,\* James L. White, Wei Zhou, Vitalie Stavila, Leonard E. Klebanoff and Terrence J. Udovic

Neutron vibrational spectroscopy and DFT calculations are used in order to gain deeper insights into the structure-dependent vibrational properties of  $\text{Mg}(\text{BH}_4)_2$  polymorphs.



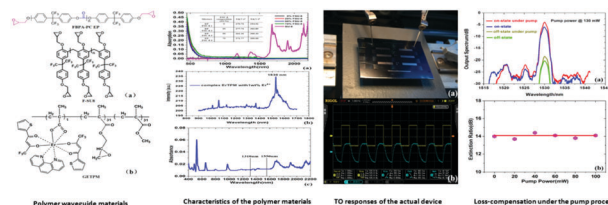
Identification of  $\text{Mg}(\text{BH}_4)_2$  polymorphs

25553

### Fluorinated photopolymer waveguide thermo-optic switches with loss-compensation function based on erbium-containing cladding structure

Yang Zheng, Changming Chen,\* Jihou Wang, Zuosen Shi, Zhenzhen Cai, Xiaoqiang Sun, Fei Wang, Zhanchen Cui and Daming Zhang

Thermo-optic switches with loss-compensation are achieved using FBPA-PC EP and GETPM. The multi-functional device is appropriate for opti-electronic integrated circuits.

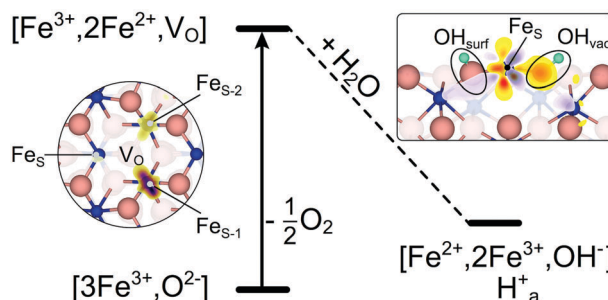


25560

### Water adsorption and O-defect formation on $\text{Fe}_2\text{O}_3(0001)$ surfaces

Roman Ovcharenko, Elena Voloshina\* and Joachim Sauer

Detailed theoretical understanding of the interaction between pristine and defective  $\alpha\text{-Fe}_2\text{O}_3(0001)$  surfaces and an isolated water molecule.

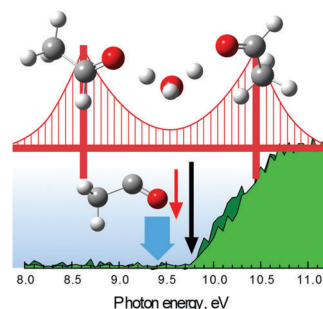


25569

### Proton transfer in acetaldehyde–water clusters mediated by a single water molecule

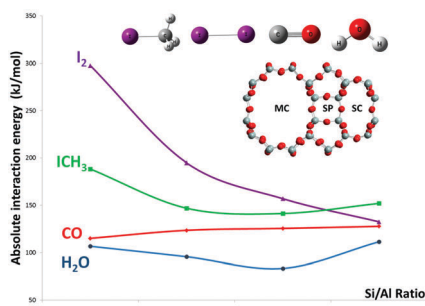
Oleg Kostko,\* Tyler P. Troy, Biswajit Bandyopadhyay and Musahid Ahmed

Bridging molecules: a single water molecule enhances the stability of symmetric acetaldehyde water clusters, and acts as a bridge for the transport of a proton between two acetaldehyde molecules.



## RESEARCH PAPERS

25574

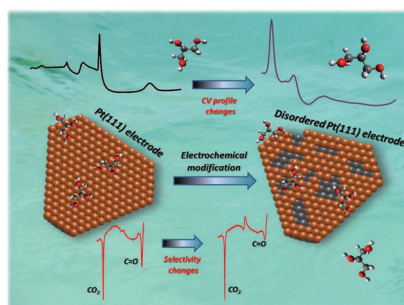


### Impact of the Si/Al ratio on the selective capture of iodine compounds in silver-mordenite: a periodic DFT study

Siwar Chibani,\* Mouheb Chebbi, Sébastien Lebègue, Laurent Cantrel and Michael Badawi\*

Decreasing the Si/Al ratio in silver exchanged mordenite drastically limits the potential inhibiting effect of H<sub>2</sub>O and CO on the adsorption of I<sub>2</sub> and ICH<sub>3</sub>, and allows a spontaneous dissociation of I<sub>2</sub> leading to the formation of AgI complexes.

25582

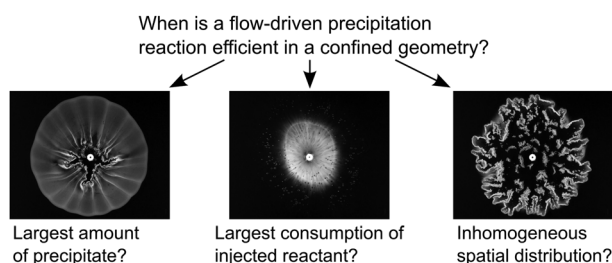


### How do random superficial defects influence the electro-oxidation of glycerol on Pt(111) surfaces?

Pablo S. Fernández,\* Polina Tereshchuk, Camilo A. Angelucci, Janaina F. Gomes, Amanda C. Garcia, Cauê A. Martins, Giuseppe A. Camara, Maria E. Martins, Juarez L. F. Da Silva and Germano Tremiliosi-Filho

The glycerol electrooxidation reaction (GEOR) has attracted huge interest in the last decade due to the very low price and availability of this polyol.

25592

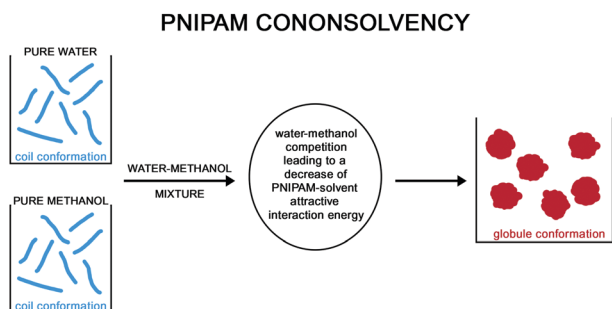


### Flow-driven control of calcium carbonate precipitation patterns in a confined geometry

Gábor Schusztar, Fabian Brau and A. De Wit\*

Upon injection of an aqueous solution of carbonate into a solution of calcium ions in the confined geometry of a Hele-Shaw cell, various calcium carbonate precipitation patterns are observed.

25601



### An alternative explanation of the cononsolvency of poly(*N*-isopropylacrylamide) in water–methanol solutions

Andrea Pica and Giuseppe Graziano\*

Water/methanol competition in the interaction with PNIPAM causes a decrease in the magnitude of attractive energy, leading to cononsolvency.

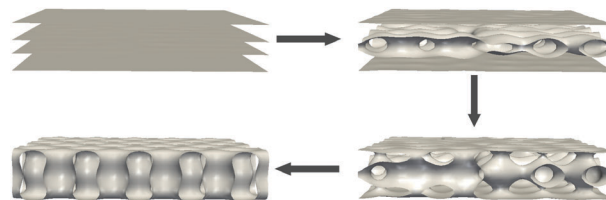
## RESEARCH PAPERS

25609

**Electric-field-induced lamellar to hexagonally perforated lamellar transition in diblock copolymer thin films: kinetic pathways**

Arnab Mukherjee,\* Kumar Ankit, Andreas Reiter, Michael Selzer and Britta Nestler

In this work, the confluence of an electric field, substrate interaction and confinement is shown to induce a parallel lamellar to hexagonally perforated lamellar transition in symmetric block-copolymer thin films.

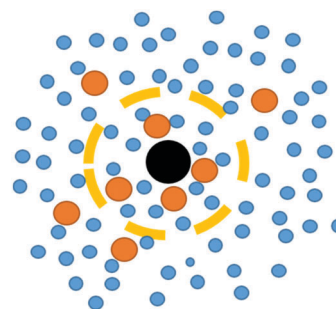


25621

**The origin of cooperative solubilisation by hydrotropes**

Seishi Shimizu\* and Nobuyuki Matubayasi

The signature of hydrotropic solubilisation is the sigmoidal solubility curve; when plotted against hydrotrope concentration, solubility increases suddenly after the minimum hydrotrope concentration (MHC), and reaches a plateau at higher hydrotrope concentrations. Here we explain the origin of hydrotropic cooperativity based on statistical thermodynamics.

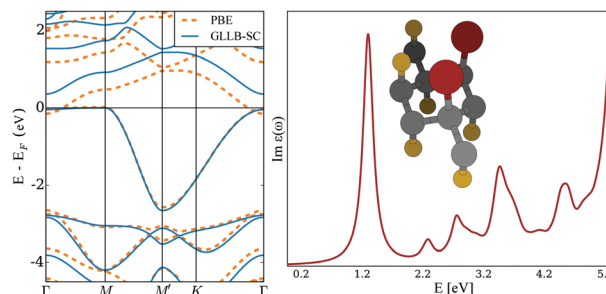


25629

**Strong 1D localization and highly anisotropic electron–hole masses in heavy-halogen functionalized graphenes**

Lukas Eugen Marsoner Steinkasserer,\* Alessandra Zarantonello and Beate Paulus

Heavy halogen functionalization of fluorographene produces systems displaying highly anisotropic charge carrier masses and optical gaps attractive for solar cell applications.

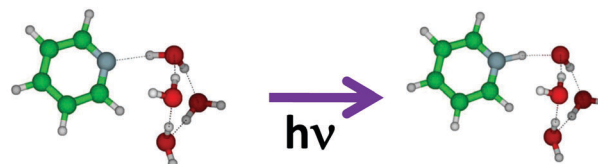


25637

**Photoinduced water splitting in pyridine water clusters**

Natalia Esteves-López, Stephane Coussan, Claude Dedonder-Lardeux and Christophe Jouvét\*

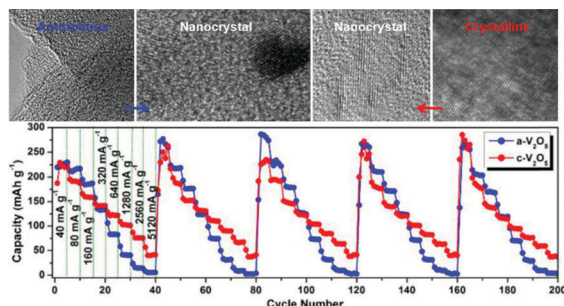
Photon induced water splitting in pyridine–(H<sub>2</sub>O)<sub>n</sub> clusters observed through the detection of the pyridinyl radical.





## RESEARCH PAPERS

25645

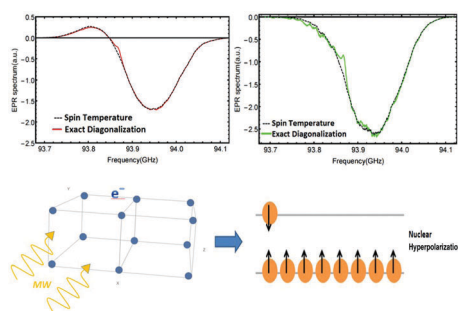


### Rational selection of amorphous or crystalline $V_2O_5$ cathode for sodium-ion batteries

Shikun Liu, Zhongqiu Tong, Jiupeng Zhao,\* Xusong Liu, Jing wang, Xiaoxuan Ma, Caixia Chi, Yu Yang, Xiaoxu Liu\* and Yao Li\*

Amorphous and crystalline  $V_2O_5$  cathodes in sodium ion batteries express inverse capacity values at low and high current densities.

25655

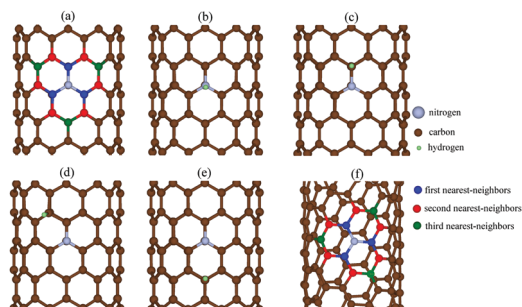


### Evidence of spin-temperature in dynamic nuclear polarization: an exact computation of the EPR spectrum

Filippo Caracciolo,\* Marta Filibian, Pietro Carretta, Alberto Rosso and Andrea De Luca

We show the validity of the spin-temperature approach for typical radical concentration used in dissolution DNP protocols.

25663

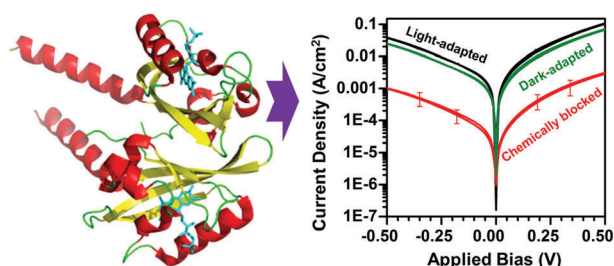


### *Ab initio* study of hydrogen chemisorption in nitrogen-doped carbon nanotubes

Julian David Correa, Elizabeth Florez\* and Miguel Eduardo Mora-Ramos

The electronic structure of single walled nitrogen-doped carbon nanotubes is calculated by first principles using density functional theory within the supercell approach with periodic boundary conditions.

25671



### Electron transport *via* a soluble photochromic photoreceptor

Sabyasachi Mukhopadhyay, Wolfgang Gärtner, David Cahen,\* Israel Pecht\* and Mordechai Sheves\*

Electron transport properties *via* a photochromic biological photoreceptor have been studied in junctions of monolayer assemblies in solid-state configurations.

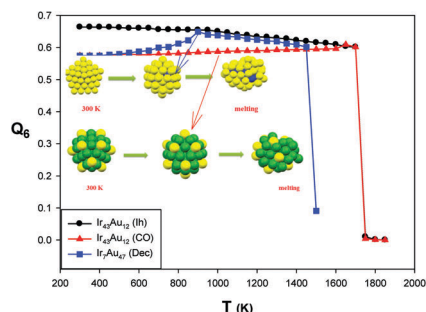
## RESEARCH PAPERS

25676

### Phase transition in crown-jewel structured Au–Ir nanoalloys with different shapes: a molecular dynamics study

Hamed Akbarzadeh,\* Mohsen Abbaspour and Esmat Mehrjouei

We have simulated the melting process for Au–Ir crown-jewel structured in the icosahedral, cuboctahedral, and decahedral morphologies.

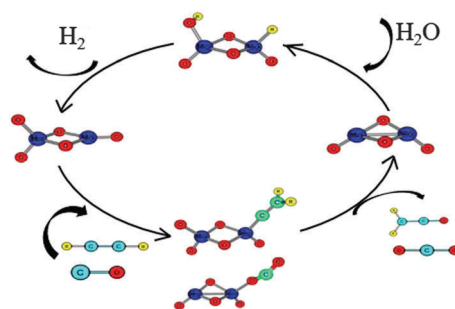


25687

### Hydrogen evolution from water using Mo–oxide clusters in the gas phase: DFT modeling of a complete catalytic cycle using a $\text{Mo}_2\text{O}_4^-/\text{Mo}_2\text{O}_5^-$ cluster couple

Manisha Ray, Arjun Saha and Krishnan Raghavachari\*

Hydrogen evolution from water using sacrificial reagents and Mo–oxide cluster anions has been explored. The internal energy preservation within the clusters plays a key role in the catalytic cycle.

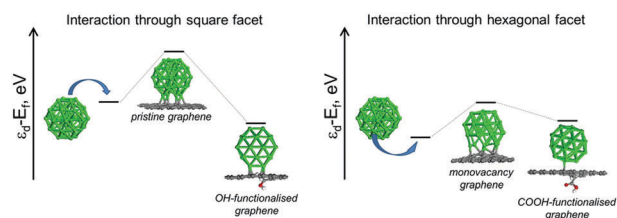


25693

### $\text{Pt}_{38}$ cluster on OH- and COOH-functionalised graphene as a model for Pt/C-catalysts

M. Matsutsu, M. A. Petersen and E. van Steen\*

Shift in d-band centre of facet of  $\text{Pt}_{38}$ -clusters opposite facet interacting with functionalised graphene indicate effect of support on reactivity.

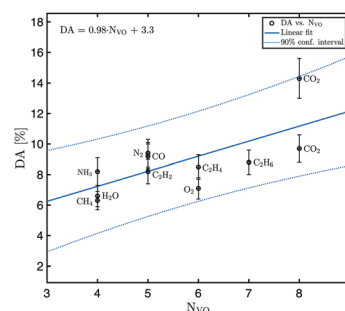


25705

### Relative extent of double and single Auger decay in molecules containing C, N and O atoms

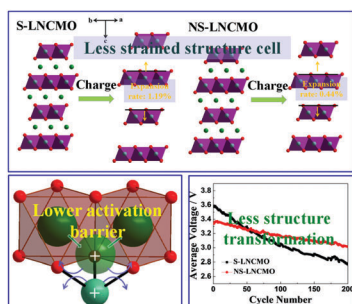
A. Hult Roos, J. H. D. Eland, J. Andersson, S. Zagorodskikh, R. Singh, R. J. Squibb and R. Feifel\*

We show that the proportion of double Auger decay following creation of single 1s core holes in molecules containing C, N and O atoms is greater than usually assumed, amounting to about 10% of single Auger decay in many cases.



## RESEARCH PAPERS

25711



### Understanding the effect of an *in situ* generated and integrated spinel phase on a layered Li-rich cathode material using a non-stoichiometric strategy

Jicheng Zhang, Rui Gao, Limei Sun, Zhengyao Li, Heng Zhang, Zhongbo Hu\* and Xiangfeng Liu\*

The effect of an *in situ* generated and integrated spinel phase on a layered Li-rich cathode material is revealed using a non-stoichiometric strategy.

25721

## Benchmark Values

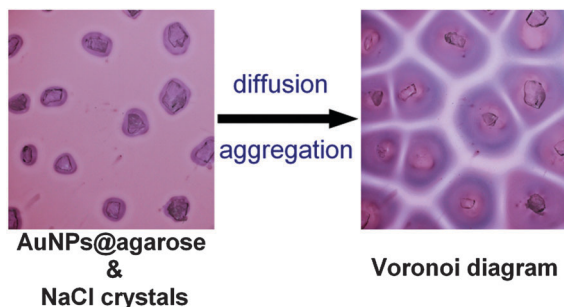
$$\mu = \frac{\partial E}{\partial N} \quad \eta = \frac{\partial \mu}{\partial N}$$

### Benchmark values of chemical potential and chemical hardness for atoms and atomic ions (including unstable anions) from the energies of isoelectronic series

Carlos Cárdenas,\* Farnaz Heidar-Zadeh and Paul W. Ayers

We present benchmark values for the electronic chemical potential and chemical hardness from reference data for ionization potentials and electron affinities.

25735

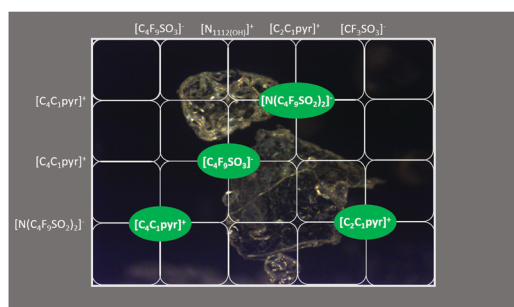


### Self-assembly of like-charged nanoparticles into Voronoi diagrams

Dániel Zámbo, Kohta Suzuno, Szilárd Pothorszky, Dóra Bárdalvy, Gábor Holló, Hideyuki Nakanishi, Dawei Wang, Daishin Ueyama, András Deák and István Lagzi\*

Diffusion and aggregation of like-charged nanoparticles can generate macroscopic patterns (Voronoi diagrams) in hydrogels.

25741



### Solid–liquid equilibria of binary mixtures of fluorinated ionic liquids

Ana Rita R. Teles, Helga Correia, Guilherme J. Maximo, Luís P. N. Rebelo, Mara G. Freire, Ana B. Pereiro\* and João A. P. Coutinho

Within ionic liquids, fluorinated ionic liquids (FILs) present unique physico-chemical properties and potential applications in several fields.

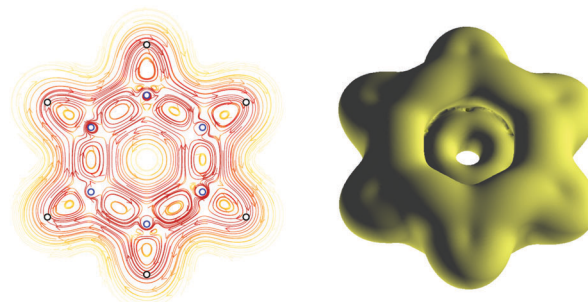
## RESEARCH PAPERS

25751

**Relativistic effects on the aromaticity of the halogenated benzenes:  $C_6X_6$ ,  $X = H, F, Cl, Br, I, At$** 

Rodrigo Ramírez-Tagle, Leonor Alvarado-Soto, Andrés Villavicencio-Wastavino and Luis Alvarez-Thon\*

We study the relativistic effects on the aromaticity of the six hexahalogenated compounds  $C_6X_6$ , via a magnetically induced current density method.

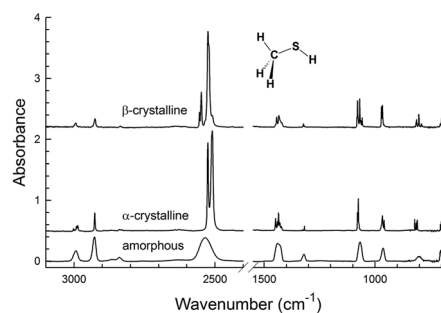


25756

**Infrared spectra and band strengths of  $CH_3SH$ , an interstellar molecule**

R. L. Hudson

Three solid phases of  $CH_3SH$  (methanethiol or methyl mercaptan) have been prepared and their mid-infrared spectra recorded at 10–110 K, with an emphasis on the 17–100 K region.



## CORRECTION

25764

**Correction: Low-field thermal mixing in  $[1-^{13}C]$  pyruvic acid for brute-force hyperpolarization**

David T. Peat, Matthew L. Hirsch, David G. Gadian, Anthony J. Horsewill, John R. Owers-Bradley\* and James G. Kempf\*